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Numerical Investigation of Aluminum Fumarate MOF adsorbent material for adsorption desalination/cooling application

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Abstract

A metal organic frame work (MOF) material called Aluminum Fumarate is numerically investigated for adsorption desalination/cooling applications in a 2-bed system and compared to silica-gel and AQSOA-Z02. Effect of evaporator and desorber bed water temperatures on cycle specific daily water production, specific cooling power and overall conversion ratio has been studied. Water temperatures ranges are (10–30°C) for evaporator and (65–85°C) for desorbing bed. It was found that for all materials, as evaporator water temperature increases, water production and cooling capacity increase. Moreover, heating source temperature has little impact on cycle performance with Al-Fumarate while when silica-gel or AQSOA-Z02 is used; cycle performance degrades dramatically with lower heating temperatures. Results showed that at 85°C hot water and 30°C evaporator and bed cooling water temperatures, Al-Fumarate can produce 11.3m³/tonne.ads/day of water and 90.9Rton/tonne.ads of cooling while AQSOA-Z02 and silica-gel produce 6.4 and 8.4m³ of water/day and cooling of 50.5 and 62.4Rton per tonne.ads respectively. Furthermore, at low bed heating water temperature of 65°C and 10°C evaporator water temperature, Al-Fumarate results in 3.4m³ of water/day and 20Rton per tonne which is 345% and 200% higher than AQSOA-Z02 and silica-gel. Therefore, Al-Fumarate has a potential in adsorption desalination-cooling applications specially at low desorption temperatures.

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Keywords: Adsorption; Desalination; Cooling; Seawater; MOF

1. Introduction

Many areas around the world are suffering from fresh water scarcity which increases the need for water desalination systems. Simultaneously with the hot and humid weather, air condition became a must for these countries. These days separate systems are used to provide cooling and fresh water through seawater desalination which consumes lots of energy and affects environments with the associated CO₂ emissions [1].

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Nomenclature

E_a	Activation energy (J.mol^{-1})	SCP	Specific cooling power ($\text{Rton.tonne.ads}^{-1}$)
W	Uptake (kg.kg^{-1})	$SDWP$	Specific daily water production ($\text{m}^3.\text{tonne.ads}^{-1}.\text{day}^{-1}$)
OCR	Overall conversion ratio (-)		

Table 1. Published work on adsorption desalination and cooling using *Silica-gel*.

Author	System used	Experiment/ Simulation	T_{hot}	SDWP ($\text{m}^3/\text{tonne ads. /day}$)	SCP (Rton/tonne ads.) @ Evap. temp. ($^{\circ}\text{C}$)
Thu et al. [2]	2 & 4 Bed	Experimental	85°C	8.79-10	0@ 30°C
Wang et al. [3]	4 Bed	Experimental	$65\text{--}85^{\circ}\text{C}$	2.5-4.7	0@ 12.2°C
Thu et al. [4, 5]	2&4 Bed, heat recovery	Exp. & Sim.	$50\text{--}85^{\circ}\text{C}$	4.27-13.5	0@ 30°C
Gong et al [6]	2 Bed with composite adsorbent	Simulation	$60\text{--}90^{\circ}\text{C}$	0	14-34@ 20°C
Uyun et al. [7]	3 Bed	Experimental	$65\text{--}80^{\circ}\text{C}$	0	16-27@ 14°C
Mitra et al. [8]	4 Bed	Experimental	85°C	2.4	18@ 5.4°C
Ng et al. [9]	2 Bed	Exp. & Sim.	85°C	7.2 3.3-4.3	46@ 30°C 20-26@ $10\text{--}15^{\circ}\text{C}$
Ng et al. [10]	4 Bed	Exp. & Sim.	85°C	8 3.6	51@ 30°C 23@ 10°C

Adsorption technology provides the solution for these needs as it is capable of producing desalinated water and cooling from the same cycle with the use of low temperature waste heat or solar energy [9].

Various cycle configurations and adsorbent materials have been applied on adsorption cycles for the production of fresh water, cooling or both. Table 1 presents different adsorption systems that were reported to produce fresh water and cooling while silica-gel is the adsorbent used.

Youssef et al. have used a new zeolite adsorbent called AQSOA-Z02 in a 2-bed [11] and 4-bed [12] adsorption desalination and cooling systems. At various desorption temperatures ($65\text{--}85^{\circ}\text{C}$) and evaporator water temperatures ($10\text{--}30^{\circ}\text{C}$) performance of silica-gel cycles was numerically compared to that of the AQSOA-Z02. For both cycles, 2 and 4 beds, it was concluded that at low chilled water temperatures below 20°C , AQSOA-Z02 outperforms silica-gel while silica-gel was found to be more suitable above 20°C . In the 4-bed cycle, AQSOA-Z02 achieved SDWP of $6.2 \text{ m}^3/\text{tonne.day}$ and SCP of 53.7 Rton/tonne compared to 3.5 m^3 of water /tonne.day and 15 Rton/tonne for silica-gel cycle using heating temperature of 85°C . In the same 4-bed system but for $T_{\text{ev}}=30^{\circ}\text{C}$, silica-gel proved to produce 9.5 m^3 of water/tonne.day and $66 \text{ Rton/tonne.day}$ which is higher than that produced by AQSOA-Z02.

Moreover, AQSOA-Z02 has been investigated by Youssef et al. [13] in a multi-cycle with integrated evaporator/condenser for the purpose of seawater desalination and cooling production using adsorption technology. Different operating modes were investigated for various combinations of desalinated water and cooling outputs according to the required outputs. The cycle configuration caused reduction in condenser temperature which enhanced system performance and resulted in maximum water production of $15.4 \text{ m}^3/\text{tonne.ads/day}$ with an improvement of 314% compared to conventional cycle when water is the only system product. However in case of water production and cooling at low evaporator temperature of 10°C , SDWP and SCP were found to be $6.64 \text{ m}^3/\text{tonne.ads/day}$ (improvement by 35%) and $46.6 \text{ Rton/tonne.ads}$ (improvement by 8.5%) respectively.

Elsayed et al. [14], have characterized and modelled three adsorbent materials from the metal organic

frameworks family namely; CPO-27Ni, Aluminum Fumarate and MIL-101Cr. Fixed adsorber bed cooling water temperature of 25°C and evaporator water temperatures of 5 and 20°C were used in the analysis with different heating temperatures in the range of (70 to 150°C). It was found that maximum water uptake for CPO-27Ni, Al-Fumarate and MIL-101Cr are 0.47gH₂O.gads-1, 0.53gH₂O.gads-1 and 1.47gH₂O.gads-1, respectively. Simulation results showed that CPO-27Ni is only suitable at high desorption temperatures above 110°C resulting in SDWP of 4.6 m³/tonne.ads/day at evaporator temperature of 5°C. At high evaporator temperature of 20°C, MIL-101 and Al-Fumarate were found to produce 11 and 6.3 m³ of water/tonne.ads/day, respectively.

From all these reviewed work, it could be noticed that the most adsorbent used in adsorption desalination/cooling cycles is silica-gel with a little contribution to AQSOA-Z02, CPO-27Ni and MIL-101Cr. Although, Al-Fumarate has been introduced into adsorption desalination applications, other operating parameters still need to be considered like adsorber bed water temperature and wider range of evaporator water inlet temperatures. In this paper, Al-Fumarate a metal organic frameworks (MOFs) material produced by Johnson Matthey is numerically investigated in a 2-bed adsorption system for the production of desalinated water and cooling. This MOF material is compared to silica-gel and AQSOA-Z02 at various desorption, adsorption and chilled water temperatures using SIMULINK modelling.

2. Mathematical Modelling

In this work, a 2-bed adsorption system is modelled using Simulink to investigate its ability to produce fresh water and cooling. In such 2-bed adsorption cycle, four main components exist which are; adsorber bed, desorber bed, evaporator and condenser as shown in figure1(a). This model simulates a full size system with each bed packed with 790 kg of a metal organic framework material called Aluminum Fumarate. Adsorbent material performance is modelled using the adsorbent isotherm model which determine maximum equilibrium uptake at certain pressure ratio and kinetics model to evaluate the corresponding uptake based on adsorption/desorption time. These two models as well as Energy, mass and salt balance equations are modelled in Simulink as per Youssef et al. [15, 16].

Adsorbent isotherms for Al-Fumarate, AQSOA-Z02 and silica-gel type RD are shown in figure 1(b) which indicates higher uptakes at pressure ratio above 0.27 for Al-Fumarate compared to silica-gel and AQSOA-Z02 [17-19]. Silica-gel isotherm is modelled using Dubinin-Astakhov (D-A) model [10], AQSOA-Z02 isotherm is modelled using the model developed by Sun et al. [19] while Al-Fumarate is modelled using polynomial and exponential expressions (equations 1-4) [18].

$$W^* = 0.111993 \exp[-0.000258797 A] \quad A > 3987 \quad (1)$$

$$W^* = 2.36129 - 9.93768E - 4 A + 1.05709E - 7A^2 \quad 2900 \leq A \leq 3987 \quad (2)$$

$$W^* = 0.5948 - 3.12E - 4 A + 1.68302E - 7A^2 - 3.124455E - 11 A^3 \quad A < 3987 \quad (3)$$

$$\text{Where } A = -RT \ln \left(\frac{P}{P_0} \right) \quad (4)$$

Adsorption kinetics are modeled by Linear Driving Force (LDF) model which is applied for the adsorbent materials, (equations 5-6) [10, 12, 18] with all constants given in table II.

$$\frac{dw}{dt} = k(w^* - w) \quad (5)$$

$$k = (15 D_{so}/R_p^2) e^{\left(\frac{-E_a}{RT}\right)} \quad (6)$$

Table 2. Linear Driving Force, LDF equation constants

Symbol	Silica gel	AQSOA-Z02		Al-Fumarate	Unit
		Pr ^b >0.1	Pr<0.1		
D_{so}	2.54 E-4	4.85 E-9	2.77 E-5	3.63 E-14	m ² /s
R_p	0.16 E-3	0.15 E-3	0.15 E-3	0.65 E-6	m
E_a	42000	17709.8	44423.5	18026	J/mol

^bPr is the pressure ratio between bed and heat exchanger

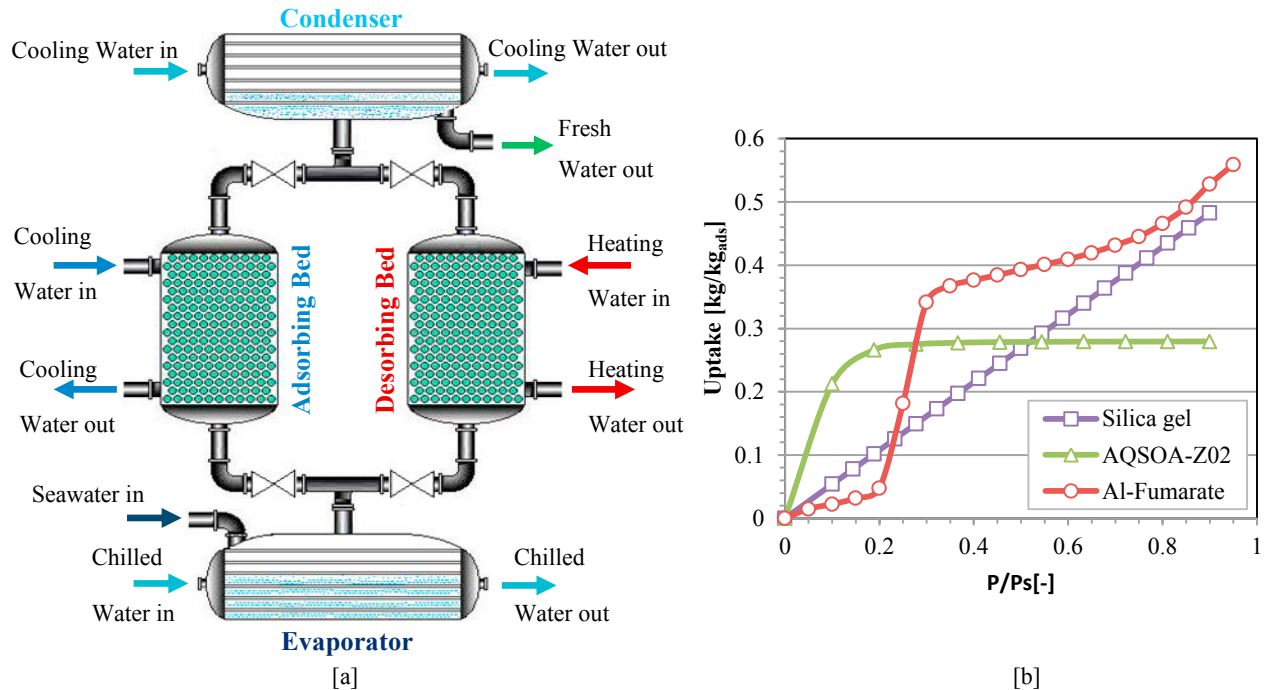


Fig. 1 (a) Schematic diagram of the adsorption system; (b) Isotherms for RD type *Silica-gel*, *AQSOA-Z02* and *AL-Fumarate*

3. Results and Discussion

This 2-bed system is investigated for different adsorption bed cooling water temperature (15–30°C), evaporator water temperature (10–30°C) and desorption bed water temperature (65–85°C) with constant condenser water temperature of 30°C and half cycle time of 425 sec. Through these parameters, cycle specific daily water production (SDWP) and specific cooling power (SCP) are compared for different adsorbent materials namely; silica-gel, AQSOA-Z02 and Al-Fumarate while cycle performance is assessed via overall conversion ratio (OCR).

Effect of desorption temperature at various evaporator water temperatures on SDWP and SCP for all materials is represented by figures 2 and 3. Three evaporator water temperatures are compared 10, 20 and 30°C which are represented by columns filled by horizontal lines, diagonal brick and vertical lines respectively. As shown in figures 2 and 3, Al-Fumarate is slightly affected by the decrease of heating water temperature from 85°C to 65°C as at evaporator water temperature of 10°C, SDWP of Al-Fumarate cycle decreases only by 1.1% from 3.47 to 3.43 m³/tonne/day. In case of silica-gel it decreases by 75% from 2.8 to 0.7 m³/tonne/day while AQSOA-Z02 decreases by 86% from 5.8 to 0.77 m³/tonne/day. For SCP and at the same conditions, Al-Fumarate cycle production decreases by 16% from 23.6 to 19.88Rton/tonne while AQSOA-Z02 cycle output decreases by 89% from 50.1 to 6.5Rton/tonne and silica-gel drops by 93% from 17.18 to 1.2Rton/tonne. Therefore Al-Fumarate cycle outperforms other cycles as it is able to operate at low heating water temperature of 65°C without big loss in output. The reason behind this performance of Al-Fumarate compared to the other two materials is the shape of isotherm uptake curves shown in figure 1(b). With the lowest slope of isotherm curve for Al-Fumarate at pressure ratios less than 0.2, changes in desorbing temperature have minimal effect on Al-Fumarate uptake unlike silica-gel and AQSOA-Z02.

For all materials, it is noticed that increasing evaporator water temperature, increases cycle outputs because of the increase in cycle uptake with the increase in the adsorption pressure ratio, fig.1(b), as it depends on evaporator temperature. As seen in figures 2 and 3 at 85°C hot water temperature, SDWP increases from 3.47 to 11.28 m³/tonne/day and SCP increases from 23.67 to 90.86Rton/tonne for Al-Fumarate when increasing evaporator water temperature from 10 to 30°C which is the maximum production compared to the other two adsorbents. Only at maximum desorbing water temperature of 85°C and lowest evaporator water temperature of 10°C, AQSOA-Z02 outperforms the other two materials as it produces 5.8 m³/day and 50.07Rton per tonne of adsorbent.

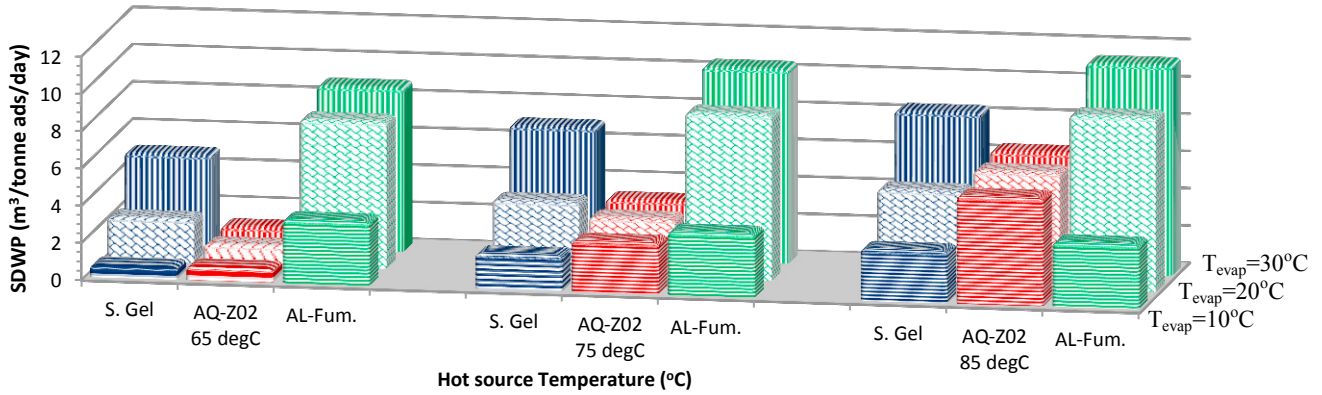


Fig. 2 SDWP of Silica-gel, AQSOA-Z02 and Al-Fumarate at different Desorption and Evaporator water temperatures

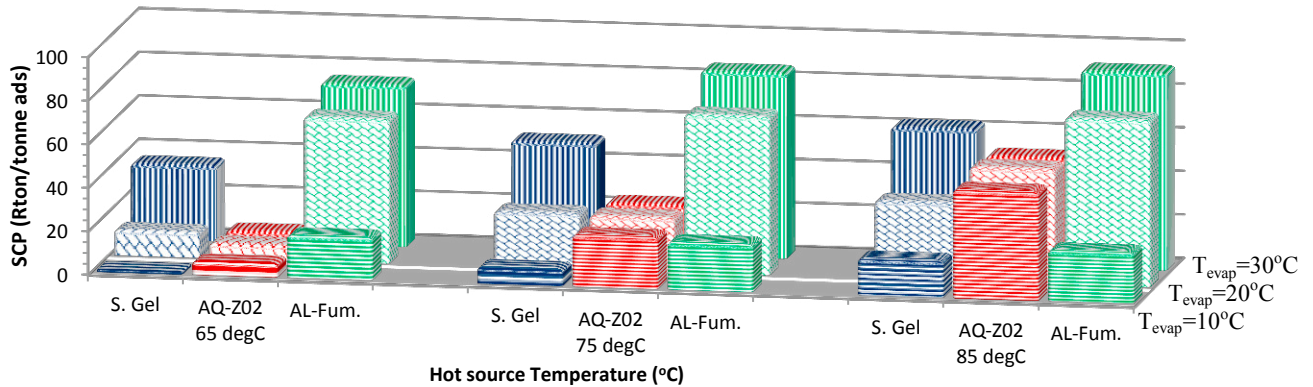


Fig. 3 SCP of Silica-gel, AQSOA-Z02 and Al-Fumarate at different Desorption and Evaporator water temperatures

Finally, these adsorbent materials are assessed in terms of OCR as in figure 4. It is observed that OCR increases by the increase in evaporator water temperature, (T_{ev}), as it ranges between 0.5 to 1 for Silica-gel and Al-Fumarate at T_{ev} of 10-30°C and hot source temperature, (T_{des}), of 85°C while for AQSOA-Z02, OCR ranges between 0.6 and 0.72. Moreover, increasing desorption temperature for silica-gel and AQSOA-Z02, increases OCR which reaches their maximum of 0.97 and 0.75 at T_{des} of 85°C respectively. However, OCR of Al-Fumarate increases with decreasing desorption temperature to reach 1.2 at T_{des} of 65°C. It is also noticed that changes in evaporator water temperature does not affect OCR of AQSOA-Z02 while for the other two materials it does. In general, OCR of Al-Fumarate is higher than all of the other adsorbent materials at all operating conditions where $T_{\text{des}} < 80^\circ\text{C}$.

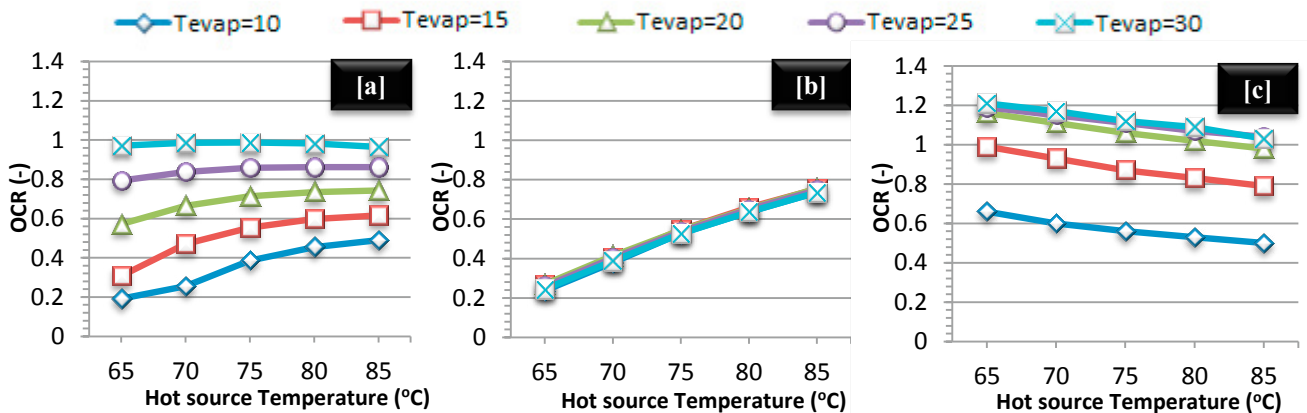


Fig. 4 OCR (a) Silica-gel, (b) AQSOA-Z02, (c) Al-Fumarate at different Desorption and Evaporator water temperatures.

4. Conclusions

An adsorbent material from the MOF family called Al-Fumarate has been numerically investigated for water desalination and cooling in a 2-bed adsorption system for water desalination and cooling purposes. Effects of desorption, adsorption and evaporator water temperatures on cycle water and cooling outputs were studied and compared to silica-gel and AQSOA-Z02. It was found that decreasing desorption temperature from 85 to 65°C has little effect on Al-Fumarate while it degrades cycle output for silica gel and AQSOA-Z02. Results showed that increasing evaporator water temperature and decreasing bed cooling water temperature increases cycle outputs for Al-Fumarate and silica-gel while it has almost no effect on AQSOA-Z02 which is reasoned by the shape of the isotherms of these adsorbents. Al-Fumarate outperformed all other materials in terms of water production and cooling at all conditions except at the lowest evaporator temperature of 10°C and at the highest bed heating temperature of 85°C where AQSOA-Z02 was better which is because of the steep increase in its uptake at low pressure ratios.

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